Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 56.8 L/kg

Global applicability domain: Inside

Local applicability domain index: 4.37e-01

Confidence level: 7.59e-01

Nearest Neighbors from the Training Set

Image not found

Nicotine
Measured: 102
Predicted: 122

Image not found

Allidochlor
Measured: 20.0
Predicted: 24.7

Image not found

Benzamide, N,N-dimethyl-
Measured: 39.8
Predicted: 36.3

Image not found

Dichlormid
Measured: 39.8
Predicted: 46.7

Image not found

N,N-Dimethylaniline
Measured: 182
Predicted: 130